Superfluid to Mott-insulator transition in an anizotropic two–dimensional optical lattice

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We study the superfluid to Mott-insulator transition of bosons in an optical anizotropic lattice by employing the Bose-Hubbard model living on a two-dimensional lattice with anizotropy parameter κ. The compressible superfluid state and incompressible Mott-insulator (MI) lobes are efficiently described analytically, using the quantum U(1) rotor approach. The ground state phase diagram showing the evolution of the MI lobes is quantified for arbitrary values of κ, corresponding to various kind of lattices: from square, through rectangular to almost one-dimensional.

1 Introduction

The type of order that a physical system can possess is utterly affected by its dimensionality. In two-dimensional ($2D$) systems with a continuous symmetry long-range order is destroyed by fluctuations at a finite temperature [1]. However, the competition between ground states in $T = 0$ can lead to a zero-temperature phase transition, driven solely by quantum mechanical fluctuations. In this context unconventional behavior in low-dimensional systems was intensively studied in the past years [2].

Since the experimental realization of Bose-Einstein condensation [3] many properties of it have been elucidated [4, 5]. Atomic gases allow clean and controlled observation of variety physical phenomena from condensed matter physics, e.g., the Berezinskii-Kosterlitz-Thouless (BKT) phase transition with the emergence of topological order [6]. The merging of atomic and condensed matter physics has opened exciting new perspectives for the creation of novel quantum states. Especially, systems of cold atoms in optical lattices [7, 8] facilitate an experimental environment, where a rich variety of quantum many-body models can be implemented in a wide range of spatial dimensions, geometries, and particle interactions. Among these topics the emergence of condensation and superfluid order in an optical lattice has been a major issue in recent years [9, 10, 11]. In this context, the presence of the optical trapping structure offers a unique way to increase (or decrease) the dimensionality of the system in a clean experimental setup, thus providing a playground for studying the effect of dimensional crossover on the quantum phase transition. This can happen in optical lattices in which atoms can tunnel easily along one spatial direction but not along the other one. This motivates the analysis of very interesting physics, e.g., of an anisotropic array of coupled one-dimensional ($1D$) Bose gases. Here, the coupling is provided by the intersite tunneling that can be made variable by adjusting the optical lattice potential. A one-dimensional situation is created by

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suppressing tunneling in two directions by using two standing waves with very high laser intensities that control the barrier between the lattice sites.

The aim of this work is to study the superfluid (SF) to Mott-insulator (MI) transition by means of the Bose-Hubbard model in $2D$ optical lattices with variable lattice anizotropy parameter. In order to quantify the evolution of the ground state phase diagram, various kind of lattices, from square, through rectangular to almost one–dimensional will be considered. To this we have adopted a theoretical approach to the strongly interacting fermions [12] in the Bose-Hubbard model in a way to include particle number fluctuations effects and make the qualitative phase diagrams more quantitative [13]. The key point of our approach is to consider the representation of strongly interacting bosons as particles with attached “flux tubes”. This introduces a U(1) phase variable, which acquires dynamic significance from the boson-boson interaction. In the present work we investigate the dimensional crossover from two- to almost $1D$ lattices and obtain the ground state phase diagram.

2 The model and method

We start with the generic model for the Mott-insulator transition, namely the Bose-Hubbard model [14]

$$\mathcal{H} = \frac{U}{2}\sum_i n_i\left(n_i - 1\right) - \sum_{\langle i,j\rangle} t_{ij} a_i^\dagger a_j - \mu \sum_i n_i, \tag{1}$$

where $a_i^\dagger$ and a_j stand for the bosonic creation and annihilation operators that obey the canonical commutation relations $[a_i, a_j^\dagger] = \delta_{ij}$, $n_i = a_i^\dagger a_i$ is the boson number operator on the site i, $U > 0$ is the on-site repulsion and the chemical potential μ controls the number of bosons. Here, $\langle i,j\rangle$ identifies summation over the nearest-neighbor sites. Furthermore, t_{ij} is the hopping matrix element with dispersion

$$t\left(\mathbf{k}\right) = 2t\left(\cos k_x + \kappa \cos k_y\right), \tag{2}$$

where κ is the anizotropy parameter and t sets the kinetic energy scale for bosons. By varying quantity κ between zero ($1D$) and one ($2D$), different anizotropic rectangular lattices emerge.

We write the partition function of the system

$$\mathcal{Z} = \int \left[\mathcal{D}\bar{a}\mathcal{D}a\right] \exp\left[-\int_0^\beta d\tau \mathcal{H}\left(\tau\right) - \sum_i \int_0^\beta d\tau \bar{a}_i\left(\tau\right)\frac{\partial}{\partial\tau} a_i\left(\tau\right)\right] \tag{3}$$

using the bosonic path-integral over the complex fields $a_i\left(\tau\right)$ depending on the “imaginary time” $0 \le \tau \le \beta \equiv 1/k_{\mathrm{B}}T$ with T being the temperature. We decouple the interaction term in Eq. (1) by a Gaussian integration over the auxiliary scalar potential fields

$$V_i\left(\tau\right) = V_{i0} + V_i'\left(\tau\right) \tag{4}$$

with static $\beta V_{i0} = V_i\left(\omega_\nu = 0\right)$ and periodic part

$$V_i'\left(\tau\right) = \beta^{-1}\sum_{\nu=1}^{+\infty} V_i\left(\omega_\nu\right)\exp\left(i\omega_\nu \tau\right) + \mathrm{c.c}, \tag{5}$$

where $\omega_\nu = 2\pi\nu/\beta$ ($\nu = 0, \pm1, \pm2, ...$) is the Bose-Matsubara frequency. Periodic part $V_i'\left(\tau\right) \equiv V_i'\left(\tau + \beta\right)$ couples to the local particle number through the Josephson-like relation

$$\dot{\phi}_i\left(\tau\right) = V_i'\left(\tau\right) \tag{6}$$

where $\dot{\phi}_i(\tau) \equiv \partial\phi_i(\tau)/\partial\tau$. The quantity $\phi(\tau)$ is the phase field satisfies the periodicity condition $\phi_i(\beta) = \phi_i(0)$ as a consequence of the periodic properties of the $V_i'(\tau)$ field. Further, we perform the local gauge transformation to the new bosonic variables

$$a_i(\tau) = b_i(\tau)\exp[i\phi_i(\tau)] \tag{7}$$

that removes the imaginary term $-i\int_0^\beta d\tau\dot{\phi}_i(\tau)n_i(\tau)$ from all the Fourier modes. From the above we deduce bosons have a composite nature made of bosonic part $b_i(\tau)$ and attached "flux" $\exp[i\phi_i(\tau)]$. Note that a similar method was used in a functional-integral formulation to treat the quantum dynamics of a microscopic model of a Josephson junction, including the dissipative effects of quasiparticle tunneling [15]. Next, we parameterize the boson fields

$$b_i(\tau) = b_0 + b_i^{'}(\tau) \tag{8}$$

and incorporate fully our in calculations the phase fluctuations governed by the gauge $\mathrm{U}(1)$ group and drop corrections to the amplitude by assuming $b_i(\tau) = b_0$, which was proven to be justified in the large U/t limit we are interested in [13, 18]. By integrating out the auxiliary static field V_{i0} we calculate the partition function $\mathcal{Z} = \int[\mathcal{D}\phi]\exp\{-\mathcal{S}_{\mathrm{ph}}[\phi]\}$, with an effective action expressed in phase-only terms

$$\mathcal{S}_{\mathrm{ph}}[\phi] = \int_0^\beta d\tau\left\{\sum_i\left[\frac{1}{2U}\dot{\phi}_i^2(\tau) + \frac{1}{i}\frac{\bar{\mu}}{U}\dot{\phi}_i(\tau)\right] - \sum_{\langle i,j\rangle}e^{i\phi_i(\tau)}J_{ij}e^{-i\phi_j(\tau)}\right\}. \tag{9}$$

We note that the phase action for the Bose-Hubbard model is closely related to the standard model of Josephson junction arrays, which contains the charging energy as well as the Josephson coupling [16, 17]. The phase stiffness coefficient is given by $J_{ij} = b_0^2 t_{ij}$, where the value

$$b_0^2 = \frac{1}{U}\left(\frac{1}{N}\sum_{\langle i,j\rangle}t_{ij} + \bar{\mu}\right) \tag{10}$$

is obtained from minimalization of the Hamiltonian $\partial\mathcal{H}(b_0)/\partial b_0 = 0$; $\bar{\mu}/U = \mu/U + 1/2$ is the shifted reduced chemical potential. The total time derivative Berry phase imaginary term in Eq. (9) is nonzero due to phase field configurations with

$$\phi_i(\beta) - \phi_i(0) = 2\pi m_i \tag{11}$$

where, $m_i = 0, \pm1, \pm2....$ Therefore, we concentrate on closed paths in the imaginary time $(0, \beta)$ labelled by the integer winding numbers m_i. The path-integral

$$\int[\mathcal{D}\phi]... \equiv \sum_{\{m_i\}}\int_0^{2\pi}[\mathcal{D}\phi(0)]\int_{\phi_i(0)}^{\phi_i(\tau)+2\pi m_i}[\mathcal{D}\phi(\tau)]..., \tag{12}$$

includes a summation over m_i and in each topological sector the integration goes over the gauge potentials. To proceed, we replace the phase degrees of freedom by the unimodular scalar complex field ψ_i which satisfies the quantum periodic boundary condition $\psi_i(\beta) = \psi_i(0)$. This can be conveniently done using the Fadeev-Popov method with Dirac delta functional resolution of unity [19], where we take ψ_i as continuous but constrained (on the average) variable to have the unimodular value

$$1 = \int\left[\mathcal{D}\psi\mathcal{D}\bar{\psi}\right]\delta\left(\sum_i|\psi_i(\tau)|^2 - N\right)\prod_i\delta\left(\psi_i - e^{i\phi_i(\tau)}\right)\delta\left(\bar{\psi}_i - e^{-i\phi_i(\tau)}\right). \tag{13}$$

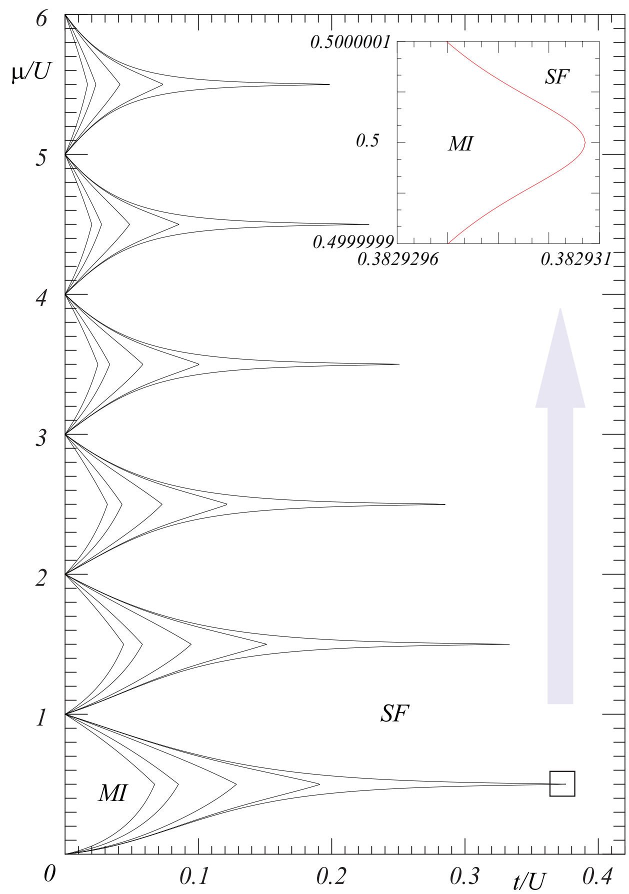

Fig. 1 (online colour) The phase boundary between the Mott insulating and superfluid phases for the anizotropic lattice with $\kappa = 1, 0.5, 10^{-1}, 10^{-2}, 10^{-5}$ from left to right. Inset shows the tip of the first lobe ($n_B = 1$) for $\kappa = 10^{-5}$.

Introducing the Lagrange multiplier λ, which adds the quadratic terms (in the ψ_i fields) to the action Eq. (9), we can solve the constraint. Using such description is justified by the definition of the order parameter

$$\Psi_B \equiv \langle a_i(\tau)\rangle = \langle b_i(\tau)\exp[i\phi_i(\tau)]\rangle = b_0\psi_B, \tag{14}$$

which non-vanishing value signals a bosonic condensation (we identify it as superfluid state). Note that a nonzero value of the amplitude b_0 is not sufficient for superfluidity. To achieve this, also the phase variables, must become stiff and coherent, which implies $\psi_B \neq 0$.

3 Phase diagram

The partition function is written in the form

$$\mathcal{Z} = \int_{-i\infty}^{+i\infty}\left[\frac{\mathcal{D}\lambda}{2\pi i}\right] e^{-N\beta\mathcal{F}(\lambda)}, \tag{15}$$

with the free energy density $\mathcal{F}=-\ln\mathcal{Z}/\beta N$ given by:

$$\mathcal{F}=-\lambda-\frac{1}{N\beta}\ln\int\left[\mathcal{D}\psi\mathcal{D}\bar{\psi}\right]\exp\left\{\sum_{i,j}\int_0^\beta d\tau d\tau'\left[\left(J\mathcal{I}_{ij}+\lambda\delta_{ij}\right)\delta\left(\tau-\tau'\right)\right]-\gamma_{ij}\psi_i\bar{\psi}_j\right\}, \quad (16)$$

where $\mathcal{I}_{ij}=1$ if i,j are the nearest neighbors and equals zero otherwise,

$$\gamma_{ij}\left(\tau,\tau'\right)=\left\langle\exp\left\{-i\left[\phi_i\left(\tau\right)-\phi_j\left(\tau'\right)\right]\right\}\right\rangle \quad (17)$$

is the two-point phase correlator associated with the order parameter field, where $\langle...\rangle$ is the averaging with respect to the action in Eq. (9). The action with the topological contribution, after Fourier transform, we write as

$$\mathcal{S}_{\text{eff}}\left[\psi,\bar{\psi}\right]=\frac{1}{N\beta}\sum_{\mathbf{k},\nu}\bar{\psi}_{\mathbf{k},\nu}\Gamma^{-1}_{\mathbf{k}}\left(\omega_\nu\right)\psi_{\mathbf{k},\nu}, \quad (18)$$

where

$$\Gamma^{-1}_{\mathbf{k}}\left(\omega_\nu\right)=\lambda-J_{\mathbf{k}}+\gamma^{-1}\left(\omega_\nu\right) \quad (19)$$

is the inverse of the propagator. The final form of the correlator, after Fourier transform, can be written as:

$$\gamma\left(\omega_\nu\right)=\frac{1}{\mathcal{Z}_0}\frac{4}{U}\sum_m\frac{\exp\left[-\frac{U\beta}{2}\left(m+\frac{\bar{\mu}}{U}\right)^2\right]}{1-4\left(m+\frac{\bar{\mu}}{U}-i\frac{\omega_\nu}{U}\right)^2}, \quad (20)$$

where

$$\mathcal{Z}_0=\sum_m\exp\left[-U\beta\left(m+\bar{\mu}/U\right)^2/2\right] \quad (21)$$

is the partition function for the set of quantum rotors. The form of Eq. (20) assures the periodicity in the imaginary time with respect to $\mu/U+1/2$ which emphasizes the special role of its integer values (see Fig. 1). Within the phase coherent state the order parameter ψ_B is evaluated in the thermodynamic limit $N\to\infty$ by the saddle point method $\delta\mathcal{F}/\delta\lambda=0$ takes the form:

$$1-\psi_B^2=\frac{1}{N\beta}\sum_{\mathbf{k},\nu}\frac{1}{\lambda-J_{\mathbf{k}}+\gamma^{-1}\left(\omega_\nu\right)}. \quad (22)$$

The phase boundary is determined by the divergence of the order parameter susceptibility $\Gamma_{\mathbf{k}=0}\left(\omega_{\nu=0}\right)=0$, which determines the critical value of the Lagrange parameter $\lambda=\lambda_0$ that stays constant in the whole ordered phase. We introduce the density of states

$$\rho\left(\xi,\kappa\right)=\frac{1}{N}\sum_{\mathbf{k}}\delta\left[\xi-t\left(\mathbf{k}\right)/t\right] \quad (23)$$

for rectangular anizotropic lattice (see inset Fig. 2):

$$\begin{aligned}\rho\left(\xi,\kappa\right) &= \frac{1}{\pi^2\sqrt{\kappa}}\mathbf{K}\left(\sqrt{\frac{\left(1+\kappa\right)^2-\xi^2}{4\kappa}}\right)\\ &\times \left[\Theta\left(\kappa-\left|\xi-1\right|\right)+\Theta\left(\kappa-\left|\xi+1\right|\right)\right]\\ &+ \frac{2\Theta\left(1-\kappa-\left|\xi\right|\right)}{\pi^2\sqrt{\left(1+\kappa\right)^2-\xi^2}}\mathbf{K}\left(\sqrt{\frac{4\kappa}{\left(1+\kappa\right)^2-\xi^2}}\right),\end{aligned} \quad (24)$$

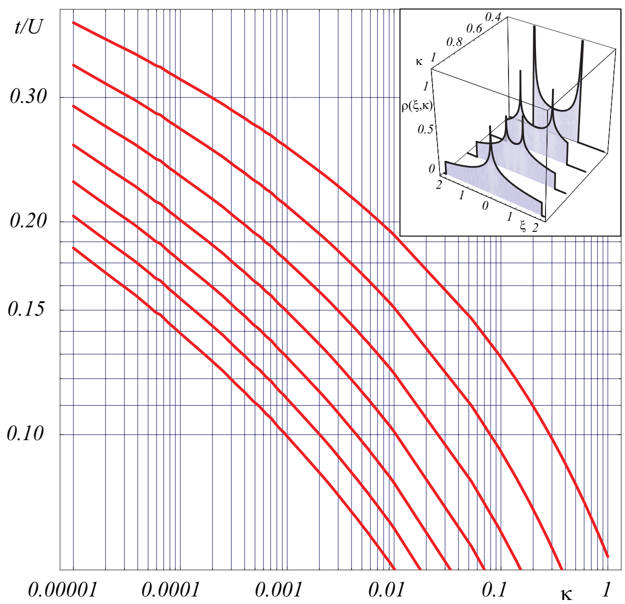

Fig. 2 (online colour) The position of the tips of the lobes as a function of the anizotropy parameter κ for $\mu/U = 0.5, 1.5, 2.5, 3.5, 4.5, 5.5, 6.5$ from right to left in double logarithmic scale. Inset shows the evolution of the density of states $\rho(\xi,\kappa)$ from square lattice ($\kappa = 1$) through rectangular ($\kappa = 0.33, 0.66$) to one-dimensional ($\kappa = 0$).

where $\Theta(x)$ is the unit step function and $\mathbf{K}(x)$ is the elliptic function of the first kind [20]. With help of the above and after summation over ω_ν, the superfluid state order parameter becomes

$$1 - \psi_B^2 = \frac{1}{2}\int_{-\infty}^{+\infty} \frac{\rho(\xi,\kappa)\, d\xi}{\sqrt{\frac{J_0 - t\xi}{U} + \upsilon^2\left(\frac{\mu}{U}\right)}}. \tag{25}$$

In Eq. (25) $\upsilon(\mu/U) = \mathrm{frac}(\mu/U) - 1/2$, where $\mathrm{frac}(x) = x - [x]$ is the fractional part of the number and $[x]$ is the floor function which gives the greatest integer less than or equal to x. The zero-temperature phase diagram of the model can be calculated from Eq. (25). We recover the results for pure $2D$ case (the lowest lobes in Fig. 1) [13]. Still there is a particle-hole asymmetry visible not in the position of the maximum of the lobe - like in simple cubic lattice - but in the shape of the curves. However, when we approach $1D$ case the particle-hole symmetry is restored. In the context of the paper [21] the existence of asymptotic restoration of the statistical particle-hole symmetry in $1D$ dirty boson problem seems to be apparent. Next, we resort to the unimodular-field description and calculate the effects of the fixed boson number

$$n_B \equiv \frac{1}{N}\sum_i \langle \bar{a}_i(\tau)\, a_i(\tau)\rangle \tag{26}$$

in the system. For the interacting problem, with the full phase action Eq. (9) we get

$$n_B = \begin{cases} n_B(\lambda) & \text{within MI phase} \\ n_B(\lambda_0) - 2\psi_B^2 \upsilon\left(\frac{\mu}{U}\right) & \text{within SF phase} \end{cases}, \tag{27}$$

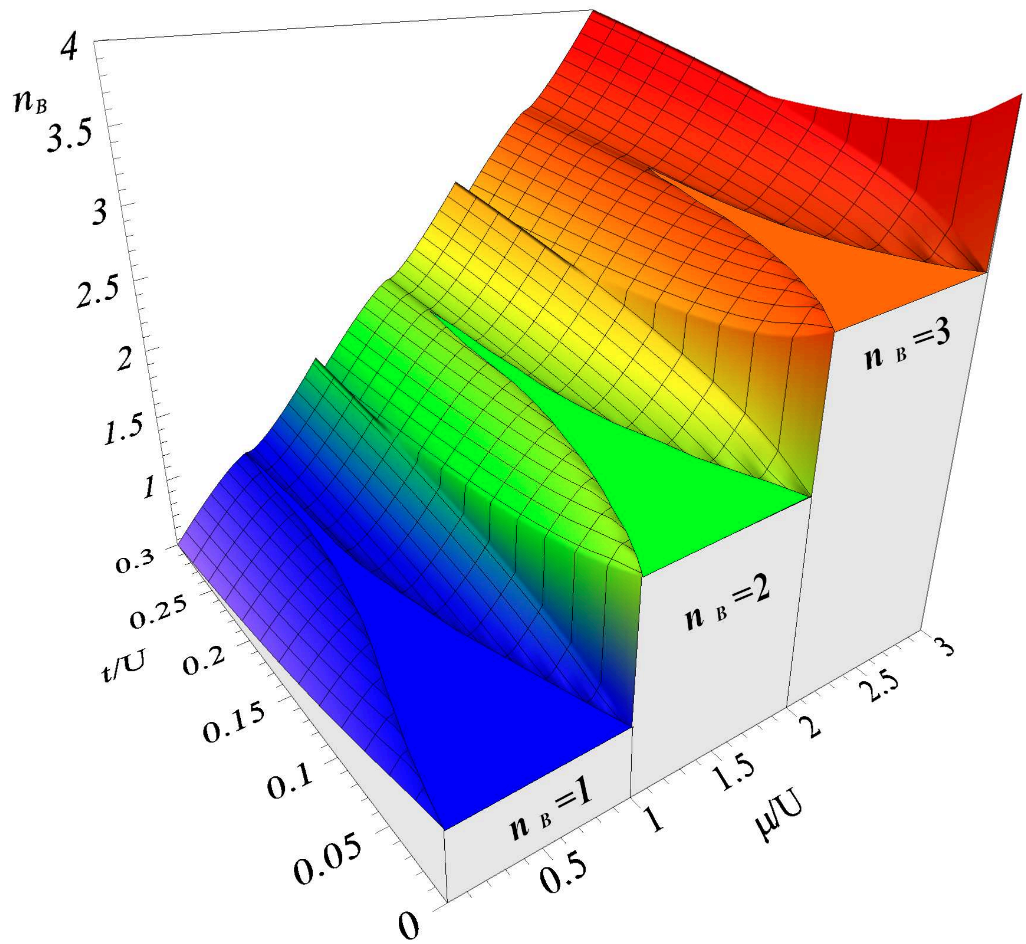

Fig. 3 (online colour) Boson occupation number n_B at $T = 0$ for the anizotropic lattice with $\kappa = 10^{-5}$ as a function of chemical potential μ/U and hopping t/U. The Mott insulator is found within each lobe of integer boson density. Inside each of MI lobe the integer occupation number n_B is indicated.

where ψ_B is given by Eq. (25). In the limit $T \to 0$ an analytical solution of the total boson density consists of the occupation number for neutral bosons n_b and a contribution δn_b from a fluctuating phase field:

$$\begin{aligned} n_B(\lambda) &= \frac{\mu}{U} + \frac{1}{2} - \upsilon\left(\frac{\mu}{U}\right) \\ &- \int_{-\infty}^{+\infty} d\xi \frac{\rho(\xi,\kappa)}{\sqrt{\frac{J_0 - t\xi}{U} + \delta\lambda + \upsilon^2\left(\frac{\mu}{U}\right)}} \end{aligned} \tag{28}$$

with $\delta\lambda = \lambda - \lambda_0$. Here, the parameter λ is self-consistently determined via Eq. (22). Changes in the anizotropy κ provide the condition for emerging MI (see Fig. 2), with recognizable steps-like structure (Fig. 3). We cannot obtain pure $1D$ case since even in $T = 0$ long-range order is destroyed by the quantum

fluctuations. Regarding the comparision of our method with the previous appraoches, e.g., [14, 18] we note that the qualitative shape of the lobes resulting from our apprach is not the same for $2D$ and $3D$ cases, and steeper for the two-dimensional system. Furthermore, we found [13] that our results are in good agreement with the recently published quantum Monte Carlo calculations on three-dimensional Bose–Hubbard system [22].

4 Final remarks

In conclusion, we have performed a study of the superfluid to Mott-insulator transition of bosons in an optical anizotropic lattice by employing the Bose-Hubbard model living on a two-dimensional lattice with anizotropy parameter κ. The compressible superfluid state and incompressible Mott-insulating lobes are efficiently described analytically, using the quantum U(1) rotor approach. Our motivation comes from the fact that the development in experimental techniques of trapping and controlling quantum gases allow to investigate such phenomena by offering a platform for the exploration of highly non-trivial quantum phases and critical phenomena in dimensionality-tunable systems. The technique used in this paper can be easily extended to more general situations, including, e.g., multi-species bosonic systems. Other generalizations of the Bose–Hubbard model are of also possible by incoporating the influence of disorder.

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